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PREDICTED ELECTRONIC SHIFTS IN FLUORINATED NAPHTHALENES

S. RAMAMURTY

MATHEMATICAL PHYSICS DEPARTMENT, ANDHRA UNIVERSITY, WALTAIR

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Murrell and Longuet-Higgins (1955) developed a method of calculating inductive perturbations taking configurational interaction into account and obtained satisfactory results in the case of benzene. Using this method and the available experimental data corresponding to system I of the vapour absorption bands of α and β fluoronaphthalenes (Ramamurty and Rao, 1957), the values of the parameters A and δ have been found to be

$$A = -0.0252, \qquad \delta^2 = 0.1304$$

For the significance of A and δ reference may be made to the paper of Murrell and Longuet-Higgins (1955).

Using these values the shifts corresponding to the system in other fluorinated naphthalenes may be calculated. The values thus predicted for some of these are given below

TABLE I

	Molecule	Shift to the red in e.V.
1, 2	Fluoronaphthalene	0.0587
1, 3	,,	0.0556
1, 4	,,	0.0606
1, 2, 3	,,	0.0894
1, 2, 4	,,	0.0900
1, 2, 3, 4	,,	0.0987

Experimental work on the absorption of these and other fluorinated naphthalenes is desirable to enable a verification of the correctness of these predictions. This work is proposed to be taken up as soon as the substances become available. Full details of the calculations will be published shortly.

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